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ADVANCEMENT AND IMPLEMENTATION OF INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME) FOR AEROSPACE APPLICATIONS (Preprint)

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UNITED STATES AIR FORCE

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14. ABSTRACT
It is believed that substantial cost, schedule, and technical benefits would result from development, implementation, and validation of Integrated Computational Materials Engineering (ICME) for aerospace propulsion applications. It is also believed that such development and implementation is necessary, even essential, to ensure that materials engineering play a significant continuing role in aerospace system design and development – in fact, it is essential for all manner of materials engineering functions. Considerable effort has been expended over the past three decades developing materials, processing, and behavior models, and many models are currently employed in the industry by both engine OEMs and their suppliers. Yet, anticipated major benefits from use of such models have not been realized in terms of significantly reduced material and process development time and cost, reduced validation time and cost, or in comprehensive implementation of model-intensive advances in life prediction, such as integrated probabilistic design and life prediction methods.

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Executive Summary

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Considerable effort has been expended over the past three decades developing materials, processing, and behavior models, and many models are currently employed in the industry by both engine OEMs and their suppliers. Yet, anticipated major benefits from use of such models have not been realized in terms of significantly reduced material and process development time and cost, reduced validation time and cost, or in comprehensive implementation of model-intensive advances in life prediction, such as integrated probabilistic design and life prediction methods.

It is believed that basic technology approaches for ICME and probabilistic methods exist, and that an industry-wide plan for integration, validation, and advancement of such methods would lead to broad implementation at OEMs and suppliers, with significant benefits to the industry and its customers.

This White Paper presents a general overview of the current state of ICME related to the aerospace propulsion industry, and identifies key challenges and barriers to broad development and implementation. These include many obvious technical challenges, as well as those related to integration of models, standardization, variation, error propagation, validation, and acceptance, amongst others. A general strategy and approach was developed and recommended to address these challenges and barriers, consisting of three elements:

- Key industrial project and focus areas
- Sustained engagement of Universities and Small Businesses
- An approach for leadership, integration, and oversight of a sustained ICME effort.

Four key industrial projects and focus areas were outlined, at least two of which might be associated or aligned with currently sponsored activities. A notional five-year plan and schedule were developed to initiate an overall ICME effort. A detailed list of recommended near term action items was also generated, in the form of "next steps" toward development of a long range plan and roadmap for ICME.

Although the result of a very brief study, the authors hope that this white paper will constitute a suitable starting point for the development of detailed long range plans and roadmaps for ICME, involving the entire materials engineering community.

**AFRL White Paper
on the
Advancement and Implementation of Integrated Computational Materials
Engineering (ICME) for Aerospace Applications**

1. Introduction:

1.1 Background: Product development in today's aerospace propulsion industry is highly complex, and very expensive. Development and certification of a new commercial gas turbine engine can easily exceed $1 Billion – and is more likely to exceed $2 Billion for a large engine with a new centerline. Many hundreds, if not thousands, of "engineer-years" of effort are required, integrating and optimizing the output of many engineering disciplines. Such an enormous business commitment, with its associated risk, has driven the industry to develop and implement sophisticated processes and computational tools that facilitate a highly integrated, systems engineering approach - to optimize and select the best performance and design combination to meet the market requirement, and then to execute the development and certification program in the shortest possible time. These efforts have resulted in considerable shortening of the development and certification period, and timelines of ~ 36 to 42 months from program "launch" to certification are achievable. Even shorter timelines are possible for derivative products. Military engine development has also benefited significantly from this progress in integrated, computationally intensive engineering. Weapon system requirements always challenge the state of the art capability in multiple engineering disciplines, while simultaneously seeking reduced development cost and time. For both commercial and military engine development, there is a strong economic incentive to minimize the cost, the number of test assets, and the time required for development testing. And, of course, there is a strong desire to minimize the number of engineering changes or significant iterations required as a result of development testing.

The concurrent and systems engineering requirements, and requirement for predictable development (success on a schedule) have driven the industry to highly sophisticated, disciplined development processes and procedures. The Integrated Product Deployment (IPD) process (sometimes also referred to as Integrated Product Development) is intended to define and ensure appropriate integration and interaction of all disciplines at appropriate times during product development, and is usually combined with gated milestones for program and technical review. This process facilitates systematic integration and "flow-down" of the high level program goals and requirements to the engine module level (turbine, combustor, compressor, etc), and further down to subassemblies and individual components. Processes, analytical procedures, and criteria are highly structured, disciplined, and documented – as in "engineering standard work" (ESW) at P&W. Incorporation of new technology in a product is similarly subjected to highly structured and disciplined processes – where "technology readiness level" (TRL) is assessed relative to defined gates, and new technologies or applications must meet gated success criteria before being "boarded" in a design [1]. This combination of

processes, procedures, and gated reviews is essential to achieve new product development goals with minimum, or at least recognized, business and technical risk.

Today, the engineering disciplines for aerodynamics, performance, controls, mechanical design, and structures can be highly integrated in a systems engineering approach. Multidisciplinary optimization (MDO) can analytically iterate and optimize solutions for product performance and configuration, and there is a high degree of integration in tools that facilitate accelerated development with minimal surprises. The industry can successfully develop and manufacture a product with globally distributed design and manufacturing responsibility – incorporating partners, major subcontractors, suppliers, and highly distributed engineering resources [2].

These same practices, requirements, and expectations are applied throughout the product life cycle – for incorporation of design or manufacturing changes, new technologies, qualification of new suppliers, assessment of deviations to specifications, and of course for development of derivative products.

1.2 Motivation for Integrated Computational Materials Engineering – ICME: Many significant advances in jet engine performance and durability have been enabled by advances in the state of the art for structural metallic materials. Notable examples are the introduction of titanium alloys, development of various nickel alloys and superalloys for many critical applications, directionally solidified and single crystal nickel-based alloys for gas path components, and advanced coatings which, when combined with advanced cooling configurations, have greatly increased turbine temperature and efficiency while simultaneously increasing durability and reducing ownership costs. Today, however, the development and validation cycle for a new or derivative metal alloy or coating remains highly empirical, *development and characterization costs are high, and the time required typically exceeds the time available in the product development cycle*. The ramifications are significant: unless a material and manufacturing process are sufficiently developed and mature at the time an engine program commits to detailed design, the program either has to forgo incorporation or carry along a backup material and configuration to mitigate risk until a final decision can be made.

As with the IPD process described above, technology development generally follows disciplined, formal, gated processes to ensure risks are acceptable and understood when a new or derivative technology is boarded in an engine program. The Technology Readiness Level (TRL) process has such critical decision gates, and when applied to materials and process development programs, the gated reviews permit periodic assessment of risk vs. remaining time and investment required in order to mature the technology sufficiently to commit to its application. A simplified illustration of the IPD and TRL processes is presented in Figure 1. Note the typical time periods required for the periods of highest development investment, and also the IPD decision gate where program launch is committed. It is at this time that materials and process development for a new material should be sufficiently mature – ie: at or near TRL-6 – to be included in the detailed design phase of a new or derivative engine program. It is apparent that either materials technology programs must be initiated well in advance of defined requirements

from a specific engine program, or the pace of materials and process development must be greatly accelerated. Similar requirements for acceleration and reduced cost can be stated for process changes to existing materials, evaluation of non-conformances, and establishing Six-Sigma or Certified Processes – all critical functions for materials engineering today.
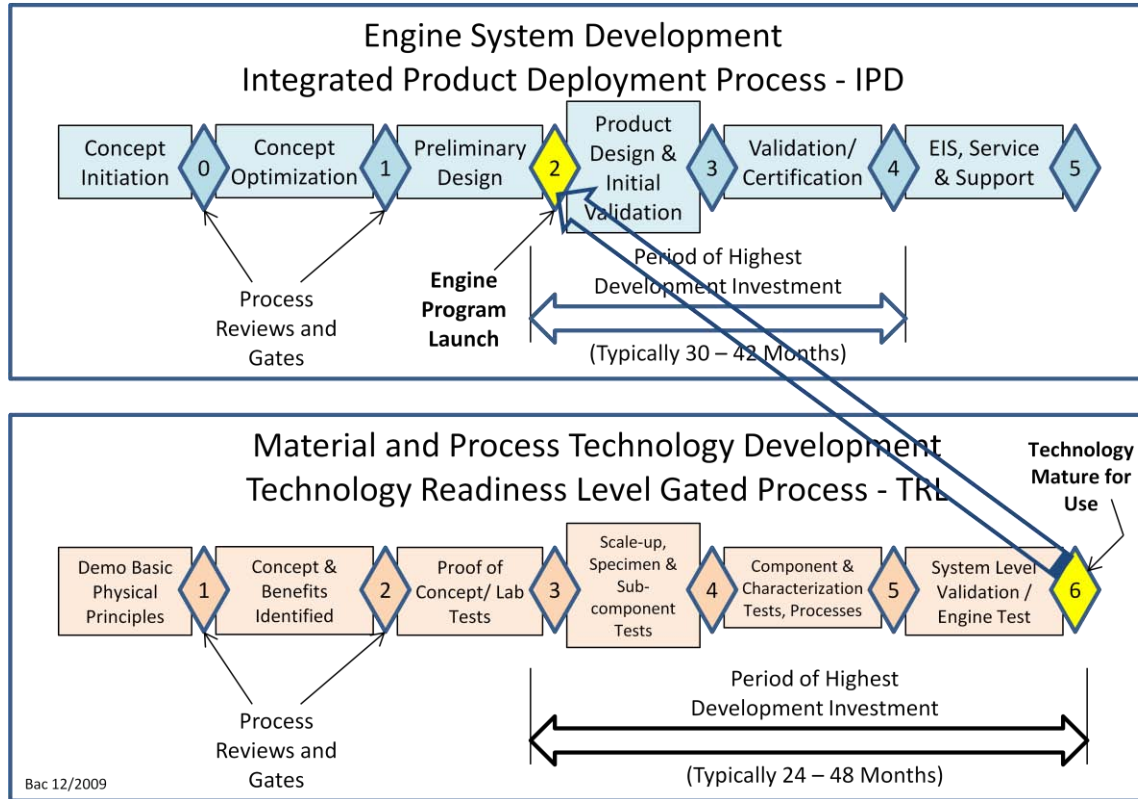
Figure 1: Schematic Representation of the IPD and TRL Processes

Considerable effort has been expended developing comprehensive materials, processing, and behavior models over the past three decades. In the early to mid-2000's, efforts were made to develop and integrate such models under the DARPA and USAF sponsored Accelerated Insertion of Materials (AIM) programs, with intent of accelerating the materials development and implementation process. There were several programs which successfully demonstrated feasibility to develop and integrate selected materials, processing, and microstructure/property models with an overall benefit to the component design and development process for the selected cases [3]. These efforts have continued and evolved over time into what is now generally referred to as "Integrated Computational Materials Engineering," or ICME.

In the broadest vision for what ICME could be, physics based computational models and requisite data bases would facilitate a fully integrated analytical representation of materials from alloy development, through process and microstructure optimization, to final physical and mechanical property prediction, in a manner suitable for integration with the aforementioned IPD process. Such capability could permit rapid material

development and characterization for insertion, as well as become an integral part of engine development and optimization analyses. With comprehensive physics-based models, new compositional or microstructural development space might be explored. Such capability would facilitate much more economical assessment of process and supplier changes, better definition of specification limits, analytical evaluation of "out-of-specification" consequences, and development of derivative or tailored materials. Understanding material property variation and its drivers could reduce characterization and validation test requirements, and facilitate maximum safe utilization of materials through more insightful probabilistic analyses and life prediction.

Many models are currently employed in the industry, by both engine OEMs and their suppliers – mostly for specific applications, and without being fully linked and integrated into the overall material, process and engine development process. Consequently, anticipated major benefits from use of such models have yet to be realized in terms of significantly reduced material and process development time and cost, reduced engine component validation time and cost, or in comprehensive implementation of model-intensive advances in life prediction, such as integrated probabilistic design and life prediction methods. It is believed that basic technology approaches for ICME and probabilistic methods exist, and that an industry-wide plan for integration, validation, and advancement of such methods would lead to broad implementation at OEMs and suppliers, with significant benefits to the industry and its customers.

2. Objectives and Scope:

Increasingly OEMs and material suppliers recognize the potential benefits of applying ICME technologies to improve and accelerate materials and process development and their application. ICME can provide clearer technical insight, enable materials and processing (M&P) optimization, achieve better quantification and management of uncertainty, while reducing the cost and delays associated with conventional experiments and testing. However, it is challenging to identify pragmatic, collaborative industrial ICME research that is technically viable at the current level of ICME maturity. Such research must provide both clear benefit and high implementation likelihood. This whitepaper addresses this difficult task.

The purpose of this document is to offer an approach to identify viable industrial ICME research projects that improve materials and processes and their application. The corresponding objectives of this whitepaper include offering:

1. A high-level overview of the current status of ICME and assessment of implementation challenges.

2. Strategies for identifying near-term research projects whose purpose and design are consistent with the current ICME maturity level, realistic opportunities for validated ICME advance, likely implementation barriers, and the need for payoff that justifies program investment.

3. Summaries for several "example projects" identified by implementing the strategy referenced above in objective #2.

If these three objectives are achieved, this whitepaper can serve as a catalyst for follow-on discussion and deliberation among government and industry stakeholders for the purpose of crafting a comprehensive, consensus plan for a funded ICME program(s).

Last year, the National Materials Advisory Board's (NMAB) Committee on Integrated Computational Materials Engineering published the results of a yearlong study to establish a vision and status assessment of ICME [4]. Based on the findings of this study, it is clear that full ICME maturation will require coordination among academia, industry, and the government, upwards to twenty years of both scientific and applied materials engineering research, transformation of materials education and the materials engineering workforce, and considerable investment. The committee's ICME vision is comprehensive, expansive, and involves the entire materials community.

The scope of this white paper is considerably more restricted. Directed by the belief that industrial practitioners and research sponsors need near-term ICME experience and project payoff, the whitepaper focuses on ICME models, tools, and project goals that can be reasonably expected to be implemented within the next five years. Although example projects, described in this document, might involve researchers from academia, industry, and the government, the associated research is intended to be pragmatic, engineering-centric, and focused upon aerospace materials and processes. Accordingly, the ensuing sections of the whitepaper will adopt a similar philosophy.

The structure of the whitepaper provides ICME background information and then applies this information to formulate a program planning strategy that is then used to identify several example ICME projects. In the next section of this study, *Background and Assessment of Current Status*, the whitepaper will present an assessment of differing perspectives of what constitutes ICME, describe the diversity of ICME users and their needs, and offer an opinion regarding the state of maturity and utility of today's suite of ICME tools and standards. The following section, *Assessment of Key Challenges and Implementation Barriers*, will attempt to outline the technical and institutional hurdles that an ICME application must overcome in order to be accepted and implemented within industry.

The information from these first two sections will then be applied in the next section, *General Strategy and Proposed Approach for an ICME Plan* by synthesizing this information and then developing an overall strategy and approach for a focused ICME plan. Specific recommended projects and activities are then described in the next section: *Recommended Elements and Focus Areas for the Proposed ICME Plan*. These key sections of the whitepaper not only outline the content and desired outcomes for the example projects but also discuss potential roles of participants. Finally, specific action items which are recommended for the near term are detailed in the following section: *Recommended Next Steps*.

Accomplishing the enumerated objectives stated above is an ambitious undertaking for this brief two-man study. However, this whitepaper does not presume to replicate earlier ICME assessments [4, 5], but instead will draw upon these earlier studies and offer ICME perspectives for near-term program ideas in a highly focused materials engineering area. Moreover, rather than attempt to formulate definitive findings, the whitepaper offers

program ideas that we hope will prove useful to the wider aerospace materials community in their efforts to define relevant industrial ICME projects.

3. Background and Assessment of Current Status

This section of the report provides an assessment of current ICME status that serves as background information to aid the formulation of viable industrial ICME applications. The assessment includes description of the ICME method, a view of the maturity of industrial relevant ICME models and tools, and finally a brief synopsis of lessons learned from prior ICME development efforts. In doing so, the report will not attempt to reanalyze ICME issues adequately covered by prior reports [4,6,7]; instead, the whitepaper will reference these reports and extend discussion only for issues of greatest relevance to ICME application by the aerospace industry.

ICME is a nascent, immature discipline and undoubtedly even the concept has varied interpretations within the materials community. While some material scientists view it as a new paradigm describing a better way to build and represent knowledge, almost all cognizant industrial materials engineers hope to exploit the concept to solve problems and replace costly and time consuming experimentation and testing. Based on the operational definition of ICME adopted by the recent NMAB study given in the text-box below, ICME rightly captures both near and farther term ICME perspectives:

[The ICME] goal is to enable the optimization of the materials, manufacturing processes, and component design long before components are fabricated, by integrating the computational processes involved into a holistic system. ICME can be defined as the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation. ... The emphasis in ICME is on the "I" for integrated and "E" for engineering. Computational materials modeling is a means to this end. [4]

As stated in this definition, the application of ICME is an engineering endeavor involving integrated modeling. In this context, integrated modeling can mean model integration across differing length and time scales for a given phenomena or simply integrated modeling among processing, microstructural evolution and properties. Furthermore, as an engineering strategy, ICME has been intended to solve problems involving the design and production of materials for engineered products.

The ICME vision espoused in prior research has encompassed a diversity of different integration architectures and software implementations [4]. One example of an ICME architecture is shown in Figure 2. The system consists of a suite of models, a database, systems analysis tools, and a graphical user interface all linked and managed via an integration software system.

Modeling

Mechanical engineering has enjoyed a strong mathematical foundation since its inception; so not surprisingly, the development of the finite-element-method (FEM) and modern computers has radically transformed the discipline. Indeed, today the FEM framework is applied to carryout sophisticated continuum heat flow, fluid flow, and structural analysis of complex geometries. Despite its predominant dependence on a single computational framework, it still has taken this discipline over 30 years to build integrated analysis systems whose application has reduced component, rig, and engine testing while reducing the product development time by a factor of three.
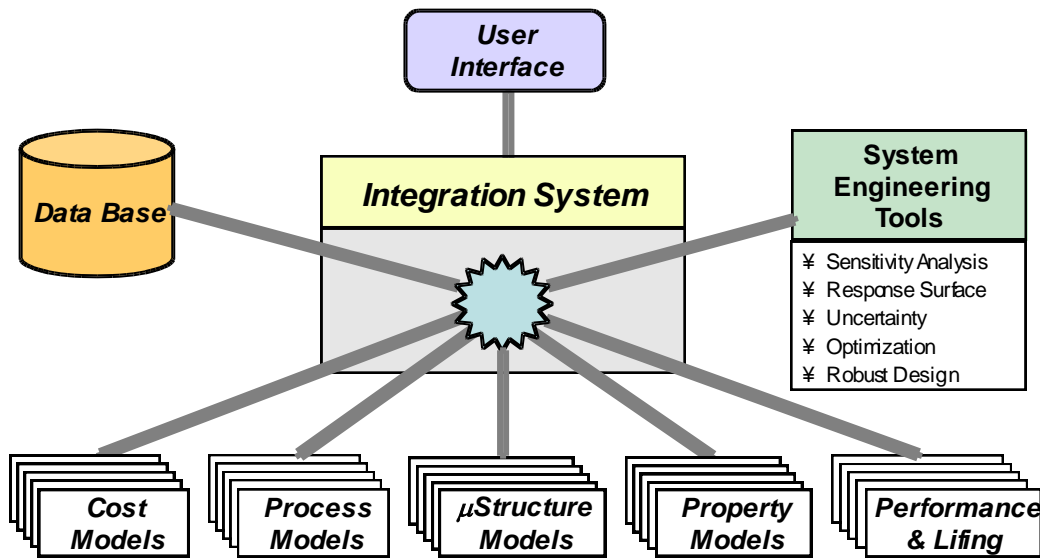
Figure 2: Pictorial representation of the typical elements of an ICME system.

Materials engineering computation has exploited these FEM advances which now serves as the backbone of casting and forging process modeling tools, such as ProCAST and DEFORM, respectively. The mathematical underpinnings of these codes are mature and the FEM implementation within these programs has been validated by comparing results with those from closed-form analytical solutions. Also, well before the ICME acronym had been coined, materials scientists and engineers were physically modeling microstructural evolution and mechanical behavior. Resulting physically based models currently used by materials scientists and engineers are listed in Table 1 [4]. This table shows the diversity of materials models, each type employing differing computational techniques, largely owing to differing length scales of the associated materials phenomena. The lack of a unifying computational technique fragments and lengthens development effort, makes validation difficult, reduces incentive for commercial code development, and requires increased specialization among materials modelers. Also, not all models in Table 1 are currently suitable for industrial application because they require excessive expertise and/or they are computationally expensive.

Table 1

Mode or Method, Required Input, Expected Output, and Typical Software Used in Materials Science and Engineering [1]			
Class of Computational Materials Model/Method	Inputs	Outputs	Software Examples
Electronic structure methods (density functional theory, quantum chemistry)	Atomic number, mass, valence electrons, crystal structure and lattice spacing, Wyckoff positions, atomic arrangement	Electronic properties, elastic constants, free energy vs. structure and other parameters, activation energies, reaction pathways, defect energies and interactions	VASP, Wien2K, CASTEP, GAMES, Gaussian, a=chem., SIESTA, DACAPO
Atomistic simulations (molecular dynamics, Monte Carlo)	Interaction scheme, potentials, methodologies, benchmarks	Thermodynamics, reaction pathways, structures, point defect and dislocation mobility, grain boundary energy and mobility, precipitate dimensions	CERIU2, LAMMPS, PARADYN, DL-POLY
Dislocation dynamics	Crystal structure and lattice spacing, elastic constants, boundary conditions, mobility laws	Stress-strain behavior, hardening behavior, effect of size scale	PARANOID, ParaDis, Dis-dynamics, Micro-Megas
Thermodynamic methods (CALPHAD)	Free-energy data from electronic structure, calorimetry data, free-energy functions fit to materials databases	Phase predominance diagrams, phase fractions, multicomponent phase diagram, free energies	Pandat, ThermoCalc, Fact Sage
Microstructural evolution methods (phase-field, front-tracking methods, Potts models)	Free-energy and kinetic databases (atom mobilities), interface and grain boundary energies, (anisotropic) interface mobilities, elastic constants	Solidification and dendritic structure, microstructure during processing, deployment, and evolution in service	OpenPF, MICRESS, DICTRA, 3DGG, Rex3D
Micromechanical and mesoscale property models (solid mechanics and FEA)	Microstructural characteristics, properties of phases and constituents	Properties of materials—for example, modulus, strength, toughness, strain tolerance, thermal/electrical conductivity, permeability; possibly creep and fatigue behavior	OOF, Voronoi Cell, JMatPro, FRANC-3D, ZenCrack, DARWIN
Microstructural imaging software	Images from optical microscopy, electron microscopes, X-rays, etc.	Image quantification and digital representations	Mimics, IDL, 3D Doctor, Amira
Mesoscale structure models (processing models)	Processing thermal and strain history	Microstructural characteristics (for example, grain size, texture, precipitate dimensions)	PrecipiCalc, JMat Pro
Part-level FEA, finite difference, and other continuum models	Part geometry, manufacturing processing parameters, component loads, materials properties	Distribution of temperatures, stresses and deformation, electrical currents, magnetic and optical behavior, etc.	ProCast, MagmaSoft, CAPCAST, DEFORM, LS-Dyna, Abaqus
Code and systems integration	Format of input and output of modules and the logical structure of integration, initial input	Parameters for optimized design, sensitivity to variations in inputs or individual modules	iSIGHT/FIPER, QMD, Phoenix
Statistical tools (neural nets, principal component analysis)	Composition, process conditions, properties	Correlations between inputs and outputs; mechanistic insights	SPLUS, MiniTab, SYSTAT, FIPER, PatternMaster, MATLAB, SAS/STAT

A second assessment, presented in Tables 2a and 2b, attempts to identify those widely available materials models that are suitable for industrial application; undoubtedly the list is incomplete. While the process models are fundamentally mature, as discussed earlier, some of the ancillary models in these modeling packages, e.g. hot tearing within ProCAST, are immature. Others such as the thermodynamic codes, Pandat and ThermoCalc, employ validated computational schemes but predictions contain error associated with errors in the thermodynamic database.

Examination of the models in Tables 2a and 2b leads to the discouraging conclusion that there is no materials-centric cost model and a dearth of microstructure and property modeling tools. Clearly, if the models described by this table were the only models available in the near future, implementation of an ICME system, like that shown in Figure 1, would be impossible for most industrial problems of interest. However, companies within the aerospace industry have internal materials models, often proprietary, based on phenomenological, statistical, and neural network methods; and more such models can be feasibly established given an accurate and properly designed dataset.

Although most materials researchers have a strong preference for physically based models, materials engineers often embrace data-driven modeling when there is a compelling need and alternatives don't exist. These engineers who adopt the so-called "80% solution" are merely acknowledging Prof. George Box's well known quote that "Essentially, all models are wrong, but some are useful" [8]. These models are useful when they serve a needed purpose and are formulated based on high quality data, employ relevant modeling forms and variables, are statistically significant, and finally model accuracy, precision, and region of applicability are rigorously determined.

Cost modeling is usually under-appreciated as an important element within the suite of material models [7] and many times it is totally ignored. Too often engineers either assume that material improvements will outweigh any added costs or they totally ignore cost implications thereby potentially violating a key constraint that may prevent implementation. The ability to quantitatively assess the cost impact of material and process changes during ICME analysis allows more accurate and realistic tradeoffs during material design and facilitates optimization by including manufacturing cost within the objective function. It is not imperative that the cost model fully captures all elements of manufacturing cost, as long as it provides sound estimates of cost derivatives for the elements of the material and manufacturing processes that are exercised during ICME analysis.

Table 2a: Widely Available Models Relevant to Industrial Application

(Representative listing; not complete)

Model Type & Output		Maturity	Comments
1.0 Thermodynamics	●		
Pandat, ThermoCalc, JMatPro		• Commercial Software	• Based on classical thermodynamic
Chemical free energy/activities		• Mature implementation	theory; requires purchase database
Phase diagrams		• Database is generally sound	
Thermophysical properties			
2.0 Material Processing			
Casting/Solidification			
ProCAST, Magma	●	• Commercial Software	• Continuum FEM for fluid flow, heat
Mold Fill		• FEM implementation mature	flow and stress analysis
Thermal & mushy zone history		• Needs better stress elements	• Solidification models for mushy
Residual stress & distortion			zone and defect formation
Forging, & Heat Treatment			
DEFORM	●	• Commercial Software	• Large strain FEM code
Die fill & forging loads		• FEM implementation mature	
Thermal & Stress/Strains history		• HTC needs further validation	
Residual stress & Distortion			
Machining distortion			
HTC determination (from TC data)			
Dante	●	• Commercial Software	• Code represents a set of sub-routines
Thermal history		• Abaqus FEM engine mature	applied within ABAQUS
Residual stress & Distortion		• Unknown maturity for HTC	• Focused on ferrous materials
HTC determination (from TC data)		& other empirical models	• Also carburizing, and properties
3.0 Microstructure & Defects			
Pandat, ThermoCalc, JMatPro	●	• Commercial Software	• Basic solidification & precipitation
Solidification microsegregation		• Microosegregation mature	theory
Precipitation Kinetics		• Precipitation is simplified	
Dictra	●	• Commercial Software	• includes a mobility database
1D Diffusion analysis		• Mature 1-D theory	• Modeling framework/language
Homogenization		• Application to 2/3-D adds risk	for custom model building
Phase transformation			
PrecipiCalc	●	• Commercial Software	• Uses classical nucleation & growth
Precipitation Kinetics		• Mature application of theory	mean-field theory
Precipitate size distribution		• Accuracy requires calibration	• Requires thermodynamic engine
JMatPro	●	• Commercial Software	• Theory based constitutive
Superalloy γ' precipitation		• Precipitation is simplified	relations for precipitation & coarsening
ProCAST	●	• Commercial Software	• Based on solidification models linked
Microsegregation		• Defect prediction based	to FEM analysis results
Dendrite arm spacing		on mature FEM results	
Shrinkage and gas porosity		• Defect based on mature	
Hot tears		solidification theory	
Freckles (airfoils)		• Theory enhancement &	
Grain structure		better input parms needed	
DEFORM *(Commercial)*	●	• Commercial Software	• Phenomenological and cellular
Recrystallization & grain growth		• Simplified theory needs data	automaton grain models

●	Mature code	
●	Not fully mature, involving simplifed analysis or requiring calibration data	
●	Unknown maturity	

Table 2b: Widely Available Models Relevant to Industrial Application

(Representative listing; not complete)

	Model Type & Output		Maturity	Comments
4.0	**Mechanical Properties**			
	JMatPro	●	• Commercial Software	• Theory based property constitutive
	Superalloy tensile properties		• Simplified theory needs data	relationships
	Superalloy creep properties			
	Imperial College Creep Model	●	• Commercial planned	• Developed by Profs. Dyson and
	Creep deformation		• Simplified theory needs data	McLean at Univ of London
	Elevated temperature flow stress			
	Univ of Michigan Yield Model	●	• University code	• Developed by Prof. Pollock
	Yield stress for γ′ superalloys		• Simplified theory needs data	• Excel implementation
	UES Yield Model	●	• AFRL code	• Model developed by Dr. Parthasarathy
	Yield stress for γ′ superalloys		• Simplified theory needs data	• Excel model derived from
5.0	**Fracture Mechanics**			
	FASTRAN	●	• NASA originated, public. avail	• Developed at NASA by Jim Newman
	General F/M code		• Strip yield model with closure	• Newman continues devl. At Miss. St.
	NASGRO	●	• NASA originated, public. avail	• Developed at NASA by R. Forman
	Simple geom, load inter, missions		• large mat'l & K soln data base	• Commercially available thru SwRI
	AFGROW	●	• USAF originated, public. avail	• Maintained by Hardman at AFRL?
	Similar to NASGRO		• large mat'l & K soln data base	
	DARWIN	●	• Commercially available	• Continued development at SwRI
	Probabilistic, non-isothermal		• NASGRO capability, plus	• Commercially available thru SwRI
	capability		probabilistic and non-isothermal	…Craig McClung
	FRANC3D	●	• Commercially available	• Development at Cornell University
	3D, Complex geometry and path		• 3D, complex geometry & path	• Available thru Fracture Anal. Consult.
			Interfaces with commerc. codes	… Paul Wawrzynek
	Several other specialized and commercial codes available….BEASY, ZENCRACK, FADD3D, CRACK3D,…			
6.0	**Component Lifing Methods**			
	This area typically proprietary and specific to OEMs			
		●	Mature code	
		●	Not fully mature, involving simplifed analysis or requiring calibration data	
		●	Unknown maturity	

Data

There are three types of data required to develop, upgrade, and execute analyses within an ICME system. These types include: (1) data required for execution of physically based codes (e.g., thermodynamic and mobility databases), (2) data for calibrating constitutive models that feed physically based models or serve as surrogates within the ICME model library, and (3) data needed to validate constituent models and overall system performance. General comments regarding the maturity state and issues for these types of data are described below:

- Thermodynamic and mobility databases are reasonably mature. However, occasionally thermodynamic calculations appear erroneous for certain chemical elements in some alloys.

- There is no community wide database containing physical properties, thermophysical properties, or properties needed for microstructural models (e.g., APB energies, surface energies, precipitate misfit) for most of the alloys relevant to aerospace applications. While some of these properties are available via calculation with programs such as JMatPro, the uncertainty of resulting values is unknown.

- Publicly available data describing elevated temperature properties relevant to processing models (e.g., emissivity, molten metal viscosity) is limited and of unknown accuracy.

- Some process input data (e.g., surface heat transfer coefficients and forging friction coefficients) can not be directly measured but must be inferred or calculated using inverse methods that may not be fully validated.

- Validation data for some models is difficult to acquire and subject to variable accuracy. While this issue is most severe with some microstructural models (e.g., measurement of fine precipitate size distributions) it also applies to some mechanical properties (e.g., measurement of elevated temperature dwell fatigue under certain environmental conditions.

While some of these data limitations are relevant to the entire materials community, the limits are greater for the most important aerospace alloys, which are often proprietary and also may be export or ITAR controlled, limiting associated research within academia. Moreover, most research sponsors have limited interest in funding data development research despite its importance to modeling and ICME.

Systems Analysis

Commercial systems analysis software is available from several suppliers; and although this capability continues to evolve it is mature and robust for application to ICME. This software, such as provided within Dassault Systemes' iSight product, provides a robust, user-friendly suite of tools for product improvement. Features often include:

- Design of orthogonal simulation trials

- Sensitivity and trend analysis

- Methods for building response surface meta-models

- Monte Carlo methods to simulate variation and uncertainty

- Procedures for performing six sigma analyses

- Multiple optimization routines employing both classical optimization routines as well as those based on genetic algorithms and simulated annealing.

- Methods to establish robust design for processes and components

Many aerospace companies, including both OEMs and suppliers, are now using systems analysis software and undoubtedly these companies will apply their chosen systems analysis software for their ICME activities.

System Integration

Much like systems analysis software, integration software is mature and in use by all aerospace OEMs within their product design organizations. These systems allow the user to link a software module with the integration platform and then later channel information between selected programs to establish an interoperable, easily reconfigurable computational network. What this means is that once a suite of models and databases have been linked within the integration system, the user can select a subset of these and logically interconnect them, usually graphically, into a specific network configuration. The output of one program then becomes the input to the next adjacent program in the network and so on until the final output prediction is achieved. Because each "use case" (type of problem) may require a unique set of models and data configured into a unique network, user-friendly reconfigurability becomes a potent integration system feature and such "use cases" can be stored for later use.

Integration systems, such as Dassault Systemes' iSight, sometimes include systems engineering utilities and interfaces for common mechanical engineering software, e.g., Catia, Ansys, MatLab, Excel, and Ascii files. For programs that don't have pre-built interfaces, the user must create the interface which typically requires expertise with a scripting language such as TCL to establish the program interface. Unfortunately, many ICME models will require such interfacing scripts, but the script only needs to be written once and can be shared.
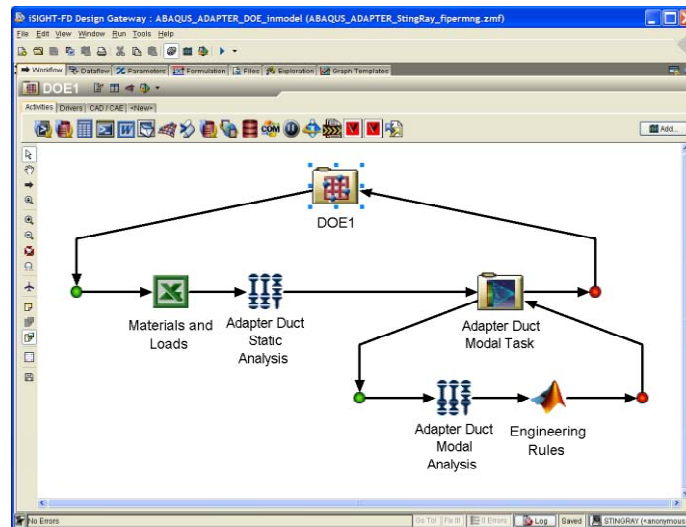

Figure 3: Systems integration showing a network of models and data within iSight.

Despite the power and importance of system integration software to build the ultimate ICME system, it is important to address how much emphasis should be given the selection and deployment of this capability in the early stages of ICME exploration

within industry. It is likely more prudent to focus development energy and resources on building and demonstrating ICME functionality and benefit for the following reasons:

- The licensing and training costs of such software can be significant;
- For those organizations that already have production software integration systems, management and IT departments will likely resist insertion of ICME modules until they are technically validated and benefit is demonstrated;
- Early application of integration software may divert manpower from more important ICME development needs; and
- Though system integration software is powerful and mature; this technology continues to advance. Future systems will likely be even better.

For those projects and organizations that choose to defer investing in system integration software, many, if not all, near-term integrated ICME applications can be integrated the old-fashion-way by piping information between software programs either manually or via scripting. Taking this approach assures that the associated ICME functionality is indeed useful and also provides integration experience that will inform the future selection of an integration software system.

Community-wide Standards

Since ICME is a nascent technology there are really no known community-wide ICME standards that promote common databases, materials representations, requirements for model verification and validation, interface standards for ICME relevant software, or even mechanisms for achieving such standards. While the materials community adheres to common ASTM standards for common modes of materials chemistry, microstructure, and property measurement and testing, members of the aerospace industry often further refine specific specification measurement techniques to reduce measurement error and improve applicability and data quality.

Early Demonstrations and Lessons Learned

The NMAB ICME report [4] contains a description of early research that developed ICME systems with integrated models, data, and systems analysis tools to demonstrate the potential benefit opportunities. Beyond providing seed ICME systems within the developing companies, these effort have been important for assessing the maturity of ICME tools, identifying key issues and challenges, and identifying pathways for ICME maturation and implementation. While this whitepaper will give a brief synopsis of two development programs, the interested reader is encouraged to refer to the NMAB ICME report for further details about these two programs and lessons learned.

In 2001 DARPA launched the Acceleration Insertion of Materials (AIM) program to apply modeling and critical data to reduce the development time for advanced aerospace materials. This goal was motivated by the expanding development cycle time gap between empirical materials development and the computational design used for product development. GE Aircraft Engines (GE) and Pratt & Whitney (P&W) collaborated to establish ICME systems supporting development of powder metallurgy turbine disk technology. These efforts used commercial software (DEFORM, ThermoCalc, Pandat, Ansys, iSight) and supported the development of PrecipiCalc and university mechanical property codes relevant to nickel-base superalloys. Both GE and P&W used iSight to

integrate these models and relevant databases and then applied the system to analyze typical test problems. P&W successfully demonstrated the ability to reduce forging weight by 21% while increasing disk burst speed by 19%; whereas GE showed how their integrated system could accelerate disk alloy development by 50%.

In the same time period, Ford Motor Company established a virtual aluminum casting (VAC) methodology to reduce the cost and time needed to develop cast automobile components. The VAC modeling system included commercial software (MagmaSoft, Pandat, Dictra, and ThermCalc) and developed a number of microstructural and property models based on the findings of in-house and funded university research. In one demonstration, Ford researchers simulated casting and heat treatment of an engine block and verified VAC predictions via comparison to measured microstructure and properties. While Ford estimates that VAC development involved 25 people and $15 million dollars, the estimated VAC return on investment was well over 7:1.

Based on the analysis conducted by the NMAB ICME committee [4], these two programs and others reviewed by the committee provide the lessons learned listed below. These lessons are self-explanatory, though further details and justification are provided in the committee report.

Lessons Learned [1]

- *ICME is an emerging discipline, still in its infancy.*

- *There is clearly a positive return on investment in ICME.*

- *Achieving the full potential of ICME requires sustained investment.*

- *ICME requires a cultural shift.*

- *Successful model integration involves distilling information at each scale.*

- *Experiments are key to the success of ICME.*

- *Databases are the key to capturing, curating, and archiving the critical information required for development of ICME.*

- *ICME activities are enabled by open-access data and integration-friendly software.*

- *In applying ICME, a less-than-perfect solution may still have high impact.*

- *Development of ICME requires cross-functional teams focused on common goals or "foundational engineering problems."*

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4. Assessment of Key Challenges and Implementation Barriers

4.1 Model Inadequacies

Without doubt, the lack of a complete suite of fully mature, validated materials models represents the greatest challenge in constructing a comprehensive ICME system. This shortcoming constricts the number and type of problems solvable using ICME, reduces

the realizable near-term payoff, and increases the risk that the fidelity of ICME predictions fall short of application needs. There are some processing and materials models that generally are considered mature, in that they implement proven and reliable algorithms. However, even these models can fall short of providing adequate accuracy owing to inaccurate embedded materials properties, constitutive property model parameters, or boundary condition values. Beyond the repercussions identifies above, the lack of mature models have the insidious effect that the repeated failure of models in practical engineering applications taints the potential value of models and builds skepticism among engineers who could otherwise become ICME advocates.

Classifying the maturity of materials and processing models is subjective at best because the accuracy and precision levels of these models are not generally available and the range of applicability is usually not specified in detail. Recognizing this caveat, Table 3 provides a condensed view of maturity for material classes based on both the perspectives and direct experience of the authors. Overall this table indicates that engineers attempting to formulate a near-term ICME system will face challenges that may temporarily require use of provisional data-driven models.

Table 3: Overview of model availability and maturity by type

	Thermo & Diffusion	Process	Defects & Microstructure	Properties
Finite Element Models		● (Mature)		
Physically-based models	● (Mature)	● (Mature)	● (Not mature)	● (Not mature)
Phenomenological Models			● (Use limited)	● (Use limited)
Statistical Models		● (Use limited)	● (Use limited)	● (Use limited)

● Mature codes available
● Not mature
● Use limited by data quality & range

4.2 Model Validation Methods and Standards

Commercial suppliers of finite-element-method (FEM) software invoke systematic methods to verify the embedded code and validate the implementation of physics within their FEM products. Validation usually entails comparison of FEM predictions against classical solutions and testing to compare results against those obtained from competing commercial software. These software suppliers often encourage and support user groups who provide feedback regarding application issues and enable continuous software improvement and better application practices.

Unfortunately, the nascent materials modeling realm does not have either agreed upon validation methods or standards whose application convey the magnitude of modeling

errors and the range of model applicability. Materials modelers lack benchmark problems whose exact solution is known or alternative widely accepted high fidelity models against which predictions can be compared. Instead, model developers usually must rely on data to test newly developed materials models. However, given the diversity of materials and processes, a model developed and validated against data from one subset of materials may not work for other materials. Model developers sometimes do provide guidance for the range of model applicability but often usually this is limited to specifying the applicable alloy class or referencing the underlying material science research upon which the model was built. Prudent model users often remain uncertain and must test the model for their particular material and process.

Developing validation methods and standards is a difficult endeavor for both cultural and technical reasons. Except for continuum mechanics FEM formulations within processing software programs, most models describing defect formation, microstructural evolution, and property development were and continue to be developed by university researchers. These researchers too often develop models to build and demonstrate understanding of operative mechanisms and have less interest in building widely applicable models for industrial application. Also, materials engineering faculty generally do not include rigorous coursework involving error determination and model validation within their curricula. Finally, increasingly university materials departments are defocusing education and research in structural materials; this change causes less appreciation for industrial modeling needs for these materials and lessened awareness of the level of model fidelity required to supplant traditional empirical, data-driven methods upon which industry has depended historically. Although it is hoped that the emergence of ICME will attract more university-industry interaction and a resurgence of industrial relevant structural materials modeling research within the academy, this transition will require significant time to acclimate university researchers to the practical engineering-based needs of the industrial materials community.

From a technical perspective, model validation is difficult because materials processing, microstructural evolution, and property development entails a rich mix of length and time scales with a equally complex set of interacting phenomena and mechanisms. There are presently no physically based models that incorporate all such phenomena and mechanisms. Instead, currently applicable models introduce simplification, homogenization, and only those mechanisms deemed dominant. Other usable models are only loosely based or inspired by mechanisms including those generally described as phenomenological or constitutive.

Because most currently applicable models do not include all relevant physics, they depend on not only physical properties that can be measured by independent measurement but also calibration (tuning) parameters that depend on the specific material and process under consideration. These calibration parameters must be deduced by comparing model prediction against corresponding experimental results; and of course the range of applicability of the parameters determined in this way depend sensitively on the specific material and process used for the experiment. Therefore, model error varies from one application to the next and depends on the suitability of the model assumptions and constitutive forms, the quality of experimental data and how well calibration parameters are determined, and the skill of the analyst who applies the model. Beyond

these difficulties, engineers who adapt these models rarely generate independent validation data sets to confirm model adequacy, calculate accuracy, and identify potential error sources. Even when a validation data set is produced and applied, the range of model applicability is limited by the range on input model parameters contained within the data set. Materials models are often non-linear and therefore the extrapolative power of these models often decreases rapidly the more they depends on calibration data.

4.3 Propagation of Variation and Error Among Linked Models

When multiple models are linked to form a modeling system, errors from each model propagate through the entire chain and it is impossible to determine the level of error in the system output without additional analysis. Even when the accuracy and precision of each model in the modeling system are seemingly reasonable, the assembly of models can produce unacceptably inaccurate and imprecise modeling results when errors compound and some models have "high gain". When the accuracy and precision of each model is unknown, reliance on the integrated modeling system introduces significant risk.

Materials and processes are also subject to variation in input variables such as chemistry, process temperature, cooling rates etc. Although each set of input parameters will produce a single deterministic output, it is often important to understand how variation of input (e.g., process) variables affects the variation in the model output (e.g., properties). Much like the propagation of errors, input variable variation propagates through a series of linked models in a way that depends on the effective gain of each model.

Monte Carlo analysis is a widely used method to track the propagation of error and variation through a system of integrated models. Application of this technique requires knowledge of the statistical distribution of model input variables, uncertain internal model parameters, and possibly other errors associated with the model formulation or the solver. The method then repeatedly selects random values and parameters from each probability distribution and executes the system of models. After a large number of such iterations, the statistical analysis of output values provides an estimate for output variation associated with error and/or input variation. When the execution time for the modeling system is sufficiently fast, the analyst can use a large number of Monte Carlo iterations thereby assuring an accurate analysis in a reasonable time. However, when the analysis includes extensive computation, such as involving FEM analysis, design engineers have demonstrated Monte Carol analysis can be accelerated by using response surfaces and approximate fast probabilistic integration methods.

4.4 Model Integration Challenges

Models within an ICME system can be integrated in a number of ways depending on the level (tightness) of integration among models and the type of communication interface(s) available for each model. Common interfacing methods include the use of application programming interfaces (API), scripts that port information between modeling programs, user defined subroutines linked to a master modeling program, and internal linkage of multiple materials models within a single program. Additionally, integration software provides preconfigured interfaces for some engineering software and utilities and procedures to facilitate integration of other software. While most materials programs (commercial or user-developed) can be linked with each other, integration often requires effort and computer expertise to translate and transfer data variables. Such efforts are

further complicated by the lack of a community-wide materials modeling standard for data exchange and the absence of a uniform materials representation for either models or databases. Below some of the common interfacing methods are briefly described.

Application Programming Interfaces – APIs are provided with many commercial engineering software programs including ABAQUS (multi-physics FEM program), MatLab (mathematical model development environment), and ThermoCalc (thermodynamic modeling program), among others. These APIs provide data formats, variable identifiers, and callable routines that allow external programs to instantiate variables, perform calculations, and retrieve resulting program output. For example, ThermoCalc provides three APIs including one that integrates MatLab and ThermoCalc and another, TQ (Thermodynamic Calculation Interface) allows an external program to retrieve thermodynamic data and perform equilibrium calculations.

Interfacing Scripts – Scripting languages such as TCL or Ruby can be used to integrate modeling software that use ASCII input/output files or have a command line interface. For this approach, the command script first executes program #1 and then retrieves the associated output file, parses and translates it to compose an input file for program #2, and so on. This approach is straightforward but also complicated and requires scripting expertise and knowledge of the individual modeling software programs to generate the command script. Also, changes to the integrated model set may require modification of the script. Despite these shortcomings, the scripting interface can be the most simple, most cost effective way to integrate models when the number is small, particularly early in the ICME development process.

User Defined Subroutines – Many commercial engineering software programs provide user defined subroutines as a way to create custom constitutive models, boundary condition functions, initialize variables, and define a user output variables. Though the allowed functionality of these subroutines is restrictive, they are a convenient and cost effective, as little programming expertise is required to utilize this method.

Internal Model Linkage within a Master Modeling Program – Major engineering modeling software often incorporates multiple models within a single program. For example, ProCast now contains not only FEM based solidification heat transfer, fluid flow and stress analysis but also a special module for continuous casting and a set of routines that predict the formation of various solidification defect types in synchronization with FEM calculations. Indeed, some materials mechanisms are coupled (e.g., the interdependence of deformation, flow stress, and precipitation during heat treat quench of a superalloy); and the best and most accurate modeling requires tightly integrated modeling such as is possible in a single modeling software package.

Commercial software suppliers will continue to add subsidiary models and features within their products to better serve their customers' needs and compete effectively with alternative suppliers. This is helpful technically, particularly when the physics of the problem demands tightly coupled solutions or when subsidiary models are fully accurate and validated. It also allows the industrial customer to license fewer commercial codes and limits training costs. However, when subsidiary models are inaccurate or unknowingly inapplicable, a user, committed to unified codes, is powerless to fully

understand the deficiency and improve the embedded code to satisfy their particular needs.

<u>Integration Software</u>

Commercial integration software, such as iSight, can be applied to integrate materials models. Also, some aerospace companies already use sophisticated integration systems to facilitate and automate their design engineering functions. iSight and Dassault Systemes' companion FIPER product can be used to create powerful computational environments that can integrate models and databases, execute system engineering processes, and provide distributed analysis and control over the internet. The use of products such as iSight or in-house systems can facilitate software integration. However, premature attempts to build a full scale integration system before ICME functionality is verified and architectural needs are confirmed, run the risk of diverting critical attention away from more pressing fundamental ICME needs (models, data generation, validation etc.) and ending up with a non-optimal ICME integration system.

4.5 Collaborative ICME Development, Intellectual Property and Export Control

ICME encompasses a broad spectrum of technologies supporting a wide variety of materials and processes. The scope is sufficiently wide that ICME development must necessarily engage the wider materials community with collaboration among companies and with academia and the government. And although construction of an ICME system involves commercial software and some models that are pre-competitive or in the public domain, collaborative development of various ICME elements will very likely encounter intellectual property, export control, and international traffic in arms regulation (ITAR) challenges. Because industrial aerospace materials researchers are familiar with these complex issues, this whitepaper will not attempt to cover them comprehensively; instead, the authors will attempt to highlight several areas of specific relevance to ICME development.

Aerospace OEMs and suppliers all protect data and processing information, which is deemed to provide competitive advantage, via patents or proprietary information control. For example, a supplier may safeguard processing methods and parameters, whereas an aerospace OEM may protect material design data and lifing methods. However, these controls can easily frustrate development of an ICME system, which depends on knowledge, data, and models that cross the boundaries between OEMs and suppliers. OEMs and suppliers must collaborate to configure information exchange in a way that precludes inverse determination of process methods or parameters while passing sufficient information to allow downstream ICME analysis. The proprietary nature of aerospace materials data also makes it difficult to assemble community wide databases because so much key mechanical property data is proprietary. However, the community can focus on building databases for common non-proprietary alloys and modeling input property data.

Interaction between ICME developers and software developers may also pose proprietary information challenges. Today many important commercial software providers are headquartered offshore (e.g., ProCAST, iSight, Abaqus, and JMatPro) and tailoring and validating embedded modules, for some export or ITAR controlled aerospace materials and processes may be challenging when transfer of controlled data is necessary.

Additionally, some software developers, domestic or foreign, have adopted business models wherein the developer retains ownership and control of future software enhancements. Though this business model is profitable for the software developer, it may impose undue long-term cost and/or hinder future enhancement for the ICME customer.

Export control and ITAR laws and regulations represent a major hurdle when interacting with domestic and foreign universities or when working with foreign companies. Most U.S. universities have sizeable numbers of international graduate students but don't have the controls and mechanisms in place to assure that non-US persons do not gain access to export or ITAR controlled information. For this reason, it is often difficult, and sometimes impossible, to engage some universities in government subcontract research having ITAR restrictions. Avoiding this challenge requires careful configuration of ICME research projects so that they avoid export and ITAR controlled technologies, possibly by confining work to theoretical issues or experiments involving similar, uncontrolled surrogate materials and processes.

4.6 Assessment and Demonstration of ICME Benefits

In the past, it has often been difficult to make a simple, conventional "business case" type of assessment for materials and process development. This has sometimes been due to the strategic nature of an enhanced material or process capability. For example, when increased operating temperature capability is enabling to a proposed product, a strategic decision to invest in enabling materials and process development might very well be made. In such cases, sponsors have invested in materials and process development with technical goals as key objectives, with a schedule constrained to meet the proposed application requirement. The "business case" is made at the product or system level, and materials and process development (if included) is a strategic element (possibly one of several) for the development program.

For the most comprehensive and inclusive future-state vision of ICME, materials and process development would be greatly accelerated, executed at reduced cost, performed without any empirical iterations, and produce results that are technically and economically superior. ICME would ideally be applicable to a broad range of relevant materials, and be applicable for a wide range of applications. Achieving such a comprehensive vision, even for select materials and applications, would require a sustained, long-term effort, and a concurrent commitment of resources for development, implementation, and validation. Such an investment will not be secured from a single sponsor, nor will it be secured at a single point in time. Rather, individual, incremental elements of an ICME capability will have to be defined, and the benefits projected in a quantified fashion – based on acceleration of schedule, reduced development iterations, reduced testing and validation, overall cost savings, reduction of risk, etc. – or more likely, some combination of these factors.

The important point is that many elements of an overall ICME system may have to be defined and assessed for merit as independent elements, in order to fit the schedule and support capability of appropriate sponsors. This leads to a later discussion in Section 6 where attributes and figures of merit are recommended for selection and assessment of proposed projects and development areas. Ideally, a standard approach for assessment of

proposed project or development efforts would be developed, consistent with an overall plan for ICME development. Such an approach would encourage, preferably require, quantitative assessment of benefits, but would not preclude identification of certain strategic elements of ICME which might not be amenable to such assessment.

4.7 Acceptance by DoD and Regulatory Agencies

The last area for commentary as a challenge for broad implementation of ICME is the acceptance of such methodology by the USAF, Navy, Army, and by regulatory agencies for commercial applications. The general area of acceptance could also be a challenge within OEMs as well, of course, for essentially the same reasons. Such acceptance has importance and may pose a challenge in at least three areas: (1) where ICME methods might affect the approach and execution of a sponsored development program, (2) where conventional testing and validation might be reduced as a result of ICME methods, and (3) where materials behavior including damage tolerance and life prediction might be affected – especially if predicted in whole or in part - by use of ICME methods.

The degree of challenge represented by each of these areas seems directly related to the level of validation and testing that would be required by the associated current, accepted, validated, and highly empirical practices. The first area cited above would likely be least challenging for these reasons – and might be acceptable with least validation of the associated ICME methods and models, since occurrence would generally be in the earlier stages of the TRL process illustrated in Figure 1, and significant testing and validation of any output would typically follow later in the TRL and IPD processes.

The more difficult challenges reside in the second and third areas described above. These areas occur later in the TRL and IPD processes shown if Figure 1, and historically have been addressed by employing significant test and validation efforts. The procedures required for validation and certification of flight engines, and any materials in critical applications within them, would certainly not be changed without substantial validation of any alternative procedure or criteria.

Consequently, the proposed strategy described later in Section 5 suggests including DoD and regulatory agency representatives in planning and review functions, to ensure up-front consideration of such issues. In addition, projects and focus areas recommended for consideration later in Section 6 were selected and described with intent to minimize or at least reduce test and validation requirements.

Ultimately, the path to achieving acceptance will likely start with the OEMs: when OEMs adopt and implement ICME methods and procedures in their "standard work," it will serve as an important endorsement for those elements of ICME.

5. General Strategy and Proposed Approach for an ICME Plan

There are many challenges and barriers to broad development and implementation of ICME, as have been previously described. Conceptually, ICME spans an extremely broad technical area, from alloy composition through complex processing and resultant microstructures, culminating with the many physical, mechanical, and life-related properties that must be determined with statistical precision. And, of course, to realize the

full potential of the ICME vision as described, the many models and facets of ICME must be integrated, validated, and compatible – not just within the materials engineering discipline, but ideally with the analytical tools of other engineering disciplines. Considering the many classes of materials, processes, properties of interest, and component applications, it seems this is a very ambitious challenge - almost overwhelming when considered in its entirety. Yet, prior programs under AIM and within various companies have demonstrated substantial benefits from an ICME approach for specific applications. Consequently, the strategy that is proposed contains short term, focused elements intended to provide opportunities to demonstrate success on key topics of interest, while generating a framework for sustainable, progressive development and implementation of ICME in the longer term.

The general strategy that is proposed in this white paper consists of three primary elements:

1. *Support and execution of selected industrial topic or focus areas,*
2. *A coordinated effort by academia and small business, and*
3. *A formal oversight and coordination activity.*

Specific considerations for these three elements follow in a later section of this document. However, before proceeding to that discussion, it is useful to consolidate and summarize the many challenges and barriers to implementation of ICME into a few, broad categories, and also to partition the elements of ICME into a few, defined focus areas:

The key challenges and barriers to broad implementation of ICME which were described in the previous section can be consolidated into a few broad categories:

Technical – *as in model capability, maturity, and available data. The recommended approach to address technical development is to select specific* *focused project* *areas where perceived benefits of ICME application would provide incentive to participants and sponsors to sustain activities and achieve success. Such selection should result in focused requirement for specific model development for each selected project.*

Integration and Standards – *meaning how various models are linked and interact, common standards for data bases and integration with other tools - especially standard commercial tools, and where interaction between companies is required. The recommended approach here includes establishment of oversight and working committees with charter to develop standards and select or designate appropriate common tools, software and data standards. It is expected that certain of the recommended project focus areas would necessitate inter-company, inter-organizational, or company-government interaction.*

Validation – *encompassing demonstrated validation protocols for accuracy, range of validity, and variation assessment, as well as assessment of error propagation especially as related to sequential application of predictive models. The recommended approach here is based on appropriate project selection to ensure that specific validation requirements are manageable.*

Acceptance by DoD and Regulatory Agencies – *such that selected, validated practices may be integrated with other analytical development, analysis, and validation tools to provide concurrent reduction in empirical test and validation*

requirements. The recommended approach here is to select appropriate project areas, and develop associated validation bases for ICME application, with the cognizance and preferably the participation of appropriate DoD and Regulatory agencies.

There were several other categories described previously as challenges and barriers to broad implementation of ICME – including benefit assessments, intellectual property, and export restrictions. It is felt that these are specific challenges that can be addressed by appropriate selection of initial topic elements, focus areas and materials, and by imposing specific "success criteria" that include formal benefit assessments for any future projects sponsored as part of a general ICME initiative. The remaining four broad areas described above must be explicitly addressed in the general strategy.

In addition, it is helpful to partition the collective concept of ICME into a few general focus areas:

Material development: alloy and composition, processing methods, microstructure, nominal properties. Note that this application would generally be early in the TRL process, and very early in the IPD process - hence less emphasis on extensive validation. Possible significant integration between supply chain and OEM companies might be required for success.

Process modeling: thermomechanical processing of specific alloy, resultant microstructure, nominal properties, process yields, residual stresses, defect species and occurrence rate. This application would generally be in the mid-to-late part of the TRL process, but still early in the IPD process – hence moderate emphasis on extensive validation. Also, significant integration between supply chain and OEM companies would be expected here, and cost modeling of material and processes would be a critical element for that interaction.

Material behavior: microstructure, properties, service aging, residual stresses, constitutive behavior and life modeling, including variation assessments, and effects of defects. This application region would be late in the TRL and possibly the IPD processes; consequently validation would become a significant requirement. Probably limited integration here between supply chain and OEM companies would be expected; but significant interaction between OEMs and USAF and/or regulatory agencies would be likely.

Although there is clearly overlap, interdependence, and redundancy amongst these three categories, they are useful to help partition the ICME universe into more manageable categories. This is helpful to determine where in the overall IPD or Technology Development Process specific ICME efforts reside. It is also helpful, possibly even essential, to assess appropriate participants and potential sponsors, required fidelity, validation requirements, and benefits that may be achieved for specific ICME development and implementation efforts.

Recognizing that ICME is very broad by nature, that ICME challenges, requirements, and benefits will vary based on focus area and specific IPD or TRL application, the general strategy that is proposed in this white paper consists of the three primary elements cited above, with intent to address the broad categories of key implementation challenges and

barriers, and to span the full application range of ICME by including material development, process modeling, and materials behavior elements.

For the near term, the proposed strategy and activities have some common features: the intent is to define and address focused project areas – developing and exercising ICME capability over a closely defined (possibly even narrow) range, minimizing the requirement for extensive experimental validation, and applying ICME modeling within a framework of existing data. For utilization of ICME in the area of alloy development, for example, the focus could be on modeling to determine the composition ranges for evaluation, with objective of rapidly and efficiently defining the alloying combinations for evaluation, and minimizing or reducing requirement for iteration. This application would by definition be early in the TRL process. Consequently, extensive validation of the ICME models would not be required in this case, as designed experiments to evaluate candidate alloys would ultimately narrow and confirm final alloy selection with experimental data. The role of ICME here would be to guide and optimize the DOX to be conducted, and ideally eliminate subsequent costly iterations that have characteristically been required in the past. "Error propagation" for such an ICME application would also be of limited concern here, since the final alloy selection would be based on actual measured properties generated for selected critical tests. Subsequent testing on the selected alloy and/or process would generate data necessary for characterization and validation.

Similarly, for evaluation of derivative materials, significant process changes to an established material, or impact of non-compliances, ICME modeling could be exercised with the goal to predict "differential" behavior, rather than absolute properties. Essentially, the goal and benefit of ICME could be to quantitatively predict change from a well-characterized baseline state of microstructure or properties, for example, rather than to predict absolute properties where extensive validation would be necessary. "Error propagation" from alloy and/or process models, to resultant microstructure and property predictions, would also be addressed by subsequent testing here, in that ICME focus would be on development of derivative material and processing, but final property determinations would still be based upon testing. Validation test requirements for such applications could be reduced or even minimized by conducting "point solution" validation tests, as an example, for selected validation of model predictions, while still providing significant savings of cost and time compared to more conventional empirical approaches commonly used today.

Validation requirements become a more central issue when ICME is applied to predict final material behavior, of course. This application by nature would occur late in the TRL process, or even late in the IPD process, where extensive data and sound statistical bases for properties are essential. The example strategy here would be to select "derivative material" applications, where extensive baseline data on a related material is already available. The ICME application here could focus on differential behavior again, and assessment of variability compared to a baseline material. Validation requirements might then be reduced through reduction of some replicate testing usually required for determination of statistical ranges, and also by use of "point solution" testing for selected validation of both mean property predictions and the statistical range. Success and confidence in the understanding of a derivative material compared to prior, established

material(s) could provide the basis for reduced component or system level validation tests, with potential for substantial cost and time savings.

We recognize that these comments on recommended approach and strategy are general in nature. The intent was to provide some general guidelines that would address what we see as the most significant challenges and barriers to broad ICME development and implementation – guidelines that would be applicable to the proposed focus and project areas, as well as the recommendations for coordination and oversight, and integration of university and small business activities.

The sections that follow offer more specific guidelines and recommendations for each or the three key elements of the proposed strategy.

6. Recommended Elements and Focus Areas for the Proposed ICME Plan

6.1 Proposed Industrial Topic or Focus Areas:

Four industrial projects and focus areas were identified and are summarized below. These focus areas are suggested as topics that are believed to offer significant, quantifiable benefits from successful application of ICME - projects that are either aligned with currently sponsored efforts, or are of high interest to various companies, especially the OEMs. In addition, it is believed that these project areas would facilitate the integration of ICME models and efforts between various companies in the overall supply chain through execution of focused projects with well-defined and manageable scope and durations. They were selected with consideration of the various challenges and barriers previously described, and attempt to span the range of ICME interest – from material and process development through and including materials behavior.

Recommended initial ICME industrial topic and focus areas:

1. ICME for Residual Stress: from processing through life management

2. ICME for Six-Sigma or Certified Processes: managing process, microstructure, and property variation, including reduced characterization and validation test requirements

3. ICME for Process Changes and Deviations: for reducing the evaluation/validation cost of planned process changes and/or unexpected deviations

4. ICME for Materials and Process Development (Derivative Materials): as in recent efforts to develop low-Re turbine airfoil alloys as derivatives from legacy alloys. Reduce time, cost, and iterations in development effort

These project focus areas and some salient features are summarized in Table 4, below. More detailed descriptions, as well as recommended objectives, scope, target materials and applications are presented later under Section 6.2.

Table 4: Summary of Recommended Industrial Project and Focus Areas

Focus Area	Title	Description	Potential Materials and Applications	Potential Lead Participants	Current Related Activity
1	ICME for Residual Stress	Bulk residual stresses from mfg assesssed & integrated with service stresses. Control and optimize for machining and performance. Utilize in component behavior assessment.	Large Ti fan or IBR-Blisk forgings; large Ni HPT disk or IBR-Blisk forgings	OEMs, Forging and Heat Treat Suppliers	AFRL DUST programs, MAI Residual Stress, AFRL workshops, supplier developments, DEFORM
2	ICME for Six-Sigma or Certified Processes	Identify, quantify and control contributors to variation in mat'ls & processes to minimize overall variation and facilitate Six-sigma or Certified Process capability.	Potential application for turbine airfoil or large structural investment castings; also any rotating component - preferrably PRP type. Also potential for any joining process - solid state or fusion.	Casting suppliers, melt sources, forging and heat treatment suppliers, OEMs.	AFRL efforts with casting suppliers, MAI on NDE for castings
3	ICME for Process Changes and Deviations	Apply ICME to process changes for established materials to facilitate new applications, adoption of alternative processes or suppliers, and analytically evaluate non-conformances.	Open. Could be aligned with project/focus areas 1 and 2 described above, or area 4 described below.	OEMs, and various supply chain companies.	Likely various - but no direct alignment identified.
4	ICME for Materials and Process Development (Derivative Materials)	Apply ICME efforts to selected aspects of derivative material & process development. Demonstrate reduced time, cost, iterations, and testing to achieve derivative.	Apply to hybrid Ni disk efforts - assess processing, microstructure, joining, projected properties vs goals	OEMs	Potential to align with AFRL and MAI programs on hybrid disk. Aligns ICME with future USAF requirements

Whether these projects are used as a basis for future ICME efforts or others are developed, it is recommended that the following guidelines be considered.

Recommended guidelines for the proposed industrial topic and focus areas:

1. Identify topic or focus area(s) that facilitate application to both wrought and investment cast product forms. Intent is to stimulate activity between OEMs, suppliers, model and code developers in what is likely to have a "process modeling" focus, as described above. Likely separate but related "tasks."
2. Ensure that a project in the "process modeling" focus area substantially addresses cost modeling. An objective should be to evaluate and/or develop standard approaches and basic modeling capability for materials and process cost modeling.
3. Identify at least one topic or focus area in "materials behavior" to address assessment of variation and validation requirements.
4. Identify a topic or focus area that addresses "material development" as described above. Limit scope to addressing the case of a "derivative material" from well-established materials or alloys.
5. Select topic or focus areas that engage multiple participants or stakeholders – such as various elements of the supply chain, OEMs, and USAF. Ensure that interaction is required to specifically address the four broad "challenges and barriers" described above.
6. In addition, it is recommended that any projects address, and be assessed against, the guidelines and attributes that are delineated later in this section, under Section 6.3.

6.2 Description of the Proposed Industrial Topic and Focus Areas

The following section presents suggested topic or focus areas along with brief descriptions including background, notional content, and general objectives. It is expected that these would be merely a starting point for discussion: there are certainly many valid considerations regarding availability of supporting information and technical difficulty, probability of success, and potential impact.

Focus Area 1: ICME for Residual Stress

Background and Notional Description: Some level of bulk and surface residual stress exists in most engine components upon completion of manufacturing and assembly. There have been many efforts to measure, control, and predict the effect of such stresses on service performance and lifetime of engine components, including current and recent efforts related to analytically treating residual stress effects and using them in subsequent component life predictions. Such capability would be especially valuable for use with rotating components such as disks, IBRs, and rotating seals. This was the subject of an AFRL sponsored workshop in 2008 and early 2009 which was facilitated by MAI [9].

What has not yet been accomplished is a systematic analysis and prediction of bulk and surface residual stresses developed during processing – predominantly forging and subsequent heat treatment and machining – which has been shown to have sufficient accuracy and predictable variation needed for use in subsequent decisions and analyses, especially those related to dimensional tolerances, burst capability, component lifing, and damage tolerance. Similar statements can be made regarding intentional residual stresses from shot peening, alternative coldworking methods, or laser shock processing. The potential impact and benefits of integrated, validated tools in this area are believed to be enormous.

Scope and Objectives: What is proposed is that a project or projects be developed that predict and perhaps optimize the processing-related bulk residual stresses for a rotor forging or IBR, including prediction of resultant residual stresses after final machining, and then utilization of these stresses in a component analysis including impact if any on burst prediction and component service life. The life prediction could be a damage tolerance assessment for buried flaw fracture mechanics; or a more aggressive application involving integration of the bulk (and surface) residual stresses with an LCF or surface damage tolerance prediction. The objectives would be to (1) integrate tools, methods, and requirements between the supply chain and the OEMs, as well as integration of manufacturing process related analyses with final engineering life predictions within the OEMs; (2) determine the relative accuracy, variability, and tolerances for the various steps where residual stress analysis would be performed, (3) employ and evaluate the various constitutive models and required input data to execute them, and (4) development of a validation protocol for such residual stresses as a function of where in the process such stress predictions would be used. It might not be possible to separate the effects of resultant microstructure on process selection, and subsequent behavior, but intent here was to focus on residual stress aspects. Also, it should be noted that the visco-plastic constitutive models required in forging analysis might differ significantly (certainly in temperature range) from the models required to assess composite stresses and their behavior over time resulting from service exposure.

Potential Target Applications and Materials: Two potential applications that would likely benefit from this focus area: (1) large titanium alloy IBRs or Blisks, where forging input weights have become very high and there is a requirement to control forging work and cooling rates to maintain desired properties, and also (2) for high pressure turbine disks, where designs for high-work single stage designs have also driven forging input weights up, and there is desire to use more complex thermal-mechanical processing to control microstructure and achieve optimum properties. In both of these examples, fracture mechanics from subsurface regions can be limiting, as well as control of dimensional growth in service. Both may be related to bulk residual stresses in the components.

Focus Area 2: ICME for Six-Sigma or Certified Processes

Background and Notional Description: One of the major challenges for ICME is that all steps in materials and process development, and ultimately all materials behavior, exhibit large intrinsic variation. The result is highly empirical, expensive, and time consuming practices to characterize and "validate" a final material process, specification, or even specific components in some cases. The goal for "Six-Sigma" controlled processes, and similar "Certified Processes" within the quality systems of some OEMs and suppliers, is to achieve highly repeatable and predictable outcomes for manufacturing processes. This requires that variation be quantified, that process capability be known, controlled and capable (in a statistical sense), and that target parameters for various processes be defined to both meet desired intent and be within such process capability. This is easily envisioned where the control parameters involve dimensional tolerances – which are readily specified and directly measurable. It is somewhat more difficult to extend this philosophy to materials and processes. It is believed that application of ICME in this area offers enormous potential benefits – in that sources of variation can be quantified, and process parameters optimized, especially for sequential processes, to achieve the desired material product with minimal statistical variation and consistently within desired target ranges for microstructure, properties, residual stresses, etc. Potential benefits would be reduced total variation in materials properties – with concurrent increases in useful minimum capability per current practices. This could have a significant impact on both primary design and life prediction properties: strength, creep, fatigue, damage tolerance. Manufacturing yields could be increased, and MRB activity minimized – ideally eliminated for Certified or Six-Sigma capable processes. And potentially the most significant benefit: either reduced total variation in material resultant properties, or quantified understanding of such variation, would lead to decreased material characterization and validation test requirements.

The inherent challenge for application of ICME in this regard: the described variation may be exacerbated by the uncertainty that accompanies any sequential or integrated application of modeling to materials engineering. Significant progress and improvement could be made here by quantifying and demonstrating understanding of variation at different stages of materials development, manufacture and characterization, as well as how variation at one step of the process propagates and affects variation at subsequent steps. A comprehensive "bottoms-up" application of ICME here would be very ambitious. However – there is considerable knowledge of how processing affects microstructure, how microstructure affects specific properties, etc., and what total

(measured) variation there is in these properties today. One small company – VexTec – has successfully developed software called VPS-Micro™ which exercises such measured properties and variation for described microstructure ranges to predict a variety of output properties and effects. This is Monte Carlo simulation software that uses empirical inputs with some level of guiding physics-based models over defined ranges.

The proposed focus area here is on quantifying, integrating, and then optimizing process parameters that contribute to variation in materials during manufacture: composition, processing, microstructure - thereby achieving a broader, more quantified understanding and prediction of final variation in the materials properties themselves.

Scope and Objectives: Development of a tractable approach for this focus area requires selection of a material, or materials, and associated processes where substantial manufacturing data already exists and is accessible for analysis. This would permit focus on analyzing and understanding measured variation, rather than having to generate it. The preferred source of this data would be from the supply chain and OEM data bases for some carefully selected materials and parts.

The scope would be to analyze and quantify the sources of variation for specific steps in the manufacturing process of the selected materials, using current data to the extent possible, and to use these results in conjunction with analytical models to predict and optimize selected process outputs. The objectives would be (1) identification and quantification of variation at various steps of material manufacturing, in terms of resulting microstructure and properties, (2) demonstration of selected models to utilize and predict such variation, and (3) use of some level of integrated models representing multiple manufacturing steps, to predict and optimize process parameters and their "target ranges" in order to achieve a more controlled and predictable product. Ideally, the result would be achievement of a "Six-Sigma" or Certified" process for the material and part production. Such tasks would involve supply chain members as well as OEMs, and the USAF or regulatory agencies if success in reducing characterization and validation requirements was indicated.

Target Applications and Materials: One example would be for titanium or nickel based rotor forgings: where it is very likely that comprehensive data bases exist for all steps of the manufacturing process, and associated material properties for the material specification as used for design. Many such rotor forgings, especially if designated a critical rotating part, have full traceability from chemistry, NDE, forging and heat treatment records, microstructure review, through integral test results, periodic cut-up test and analysis, and finally characterization for specification or blueprint requirements.

A second example would be for an investment casting – either a large structural casting or perhaps a turbine airfoil. The large structural castings are by nature lower production runs and high unit cost, where the airfoils may be very high volume, with many parts sharing specific master melts, casting pours, and subsequent heat treatments. Here the focus might be process modeling, to predict die fill, probability of defects, and resultant microstructures. Focus would be on optimizing process yields, perhaps reducing rework for large structural castings, and achieving desired properties.

Focus Area 3: ICME for Process Changes and Deviations

Background and Notional Description: Planned or required process changes and occasional deviations present an opportunity for ICME to reduce the empirical testing and validation that is currently the normal practice used for evaluation. The historical practice for process control is to achieve an acceptable process output and then "freeze" the parameters to ensure future compliance with intent. This of course can restrict opportunity to make continuous improvements, requires sometimes extensive testing, especially if a significant process change or supplier source change is made, or if a process parameter or resultant measure is out of compliance. There are several opportunities for ICME application in this area. Modeling of process parameters and their output, much like what was described for Focus Area 2 above, is certainly one area. This could be in a proactive sense to optimize or improve a process, or assess impact of a desired change. It could also be done "after the fact" – as in the case for evaluation of unexpected deviations either from prescribed process parameters or as determined from measured results (properties, microstructure). One likely advantage for this focus area: specific target materials and processes would presumably have well characterized current processes and outputs. Consequently, the ICME challenge would be bounded within or just beyond known regions for microstructure and properties. One area of interest that would likely be too aggressive for initial application: surface finish-related processes such as machining. Although these may be significant factors in cost and schedule for process changes and deviations today, it is recommended they not be addressed during initial efforts.

Scope and Objectives: Several potential refinements to this focus area to better define scope are offered: (1) application of ICME for production of a new part, one that is within a current specification but requires specific process development (like a new forging with significant configuration change or size from prior process), (2) a change in source supplier for a significant process on a current material and part, and (3) evaluation of process deviations or resultant properties for purposes of MRB evaluation and resolution. The objectives would be to (1) utilize ICME models and predictions to assess effects of process changes, (2) utilize ICME models and current data to evaluate consequences of deviations from specified processes or to evaluate non-conforming results for impact on serviceability, and (3) demonstrate reduced requirement for empirical substantiation of the above. It is envisioned that this focus area would require interaction between suppliers and OEMs, as well as between materials, manufacturing, structures, program, and quality organizations within the OEMs.

Target Applications and Materials: Target materials and applications of interest for area could be related to the projects described in both focus areas 1 and 2 previously, except scope could be limited to selected process changes or deviations. Ideally, selected materials and product forms would have significant empirical data supporting them, to facilitate evaluation and validation of ICME modeling efforts performed in support of this focus area.

Focus Area 4: ICME for Materials and Process Development (Derivative Materials)

Background and Notional Description: Certainly one long-term vision for ICME involves the ability to develop and validate a future material based on comprehensive

modeling – from initial alloy selection through various processing steps to achieve desired microstructures, and finally to achieve target properties - all with greatly reduced empirical iteration and testing along the way. The focus of this white paper has been to describe the barriers and challenges to full realization of such a vision – which are considerable. That does not preclude specific application in a more tractable manner – namely to assist development and optimization of "derivative materials." This is of course done in an empirical or semi-empirical manner today. OEMs, and select companies who undertake commercial alloy development, certainly use their established data bases, materials engineering knowledge, and selected current software and models to guide future alloy and process development programs. One recent observation supporting this: at least two engine OEMs have developed derivative single crystal alloys for turbine airfoils in much reduced time compared to typical new alloy development programs, in response to extreme increases in recent market prices for some critical and strategic alloying elements. The ability to do this, and commit to market application, is likely the result of improved (accelerated) development practices facilitated by "ICME-like" capability, to reduce development iterations, cost, time, and risk. The extent to which ICME-like methods contributed here has not been made public.

It is highly desirable to have at least one focus area involve material development. Consequently, a focus area is recommended that addresses development of a derivative material or process. One opportunity to align this with current AFRL interests would be to associate it with development of the hybrid-disk concept for future applications which require increased T3 (compressor exit temperature) and/or increased time at elevated temperature for both the compressor and high pressure turbine. Achieving necessary capability here requires improved creep, TMF, and environmental resistant of the rotor alloys at a minimum. It is likely to require novel constructs involving multiple processes (and microstructures) or even multiple alloys in the same hybrid rotor. Although AFRL support of this objective is already underway, a concurrent task related to ICME aligned with that effort would likely be beneficial and would provide focus for the ICME effort.

Scope and Objectives: Scope in this case would include focus on material development aspects not significantly included in the previously described topic areas. Scope might include alloy and phase predictions; certainly it would include microstructure predictions for complex processing and specifically any transition areas or boundaries between processing areas. The scope may include analysis of joining areas for dissimilar alloys or material forms. Objectives would include development and application of ICME models to (1) assess microstructure and properties for hybrid rotors with complex processing, (2) define processing parameters and limits for desirable results, and (3) determine and minimize required characterization and testing for resultant material with complex processing and structure.

Target Applications and Materials: Target application would be material or hybrid disk development aligned with AFRL effort for "hybrid disks." Inference is that this would involve current or next generation powder metal superalloys, with complex processing possibly involving both sub-solvus and hyper-solvus processing (referring to gamma prime phase), and possibly multiple alloys or even multiple alloy forms in the same bonded assembly.

6.3 Recommended Criteria for Candidate Industrial ICME Projects

This section contains some general attributes and success criteria that are highly recommended for consideration when evaluating any proposed project or task related to an ICME initiative. Certainly relative weighting could be developed to help assess any proposed projects depending on focus area, technical difficulty, and potential benefits if successful.

1. The project establishes ICME capability that addresses a recognized problem or material system enhancement, (e.g., reduces mfg cost, improves properties, or provides information that enhance application of the material).
2. The project develops ICME capability that upon implementation is projected to add value exceeding its recurring deployment cost.
3. The project includes an approach to quantify implementation benefit.
4. The project uses models that are mature or can be reasonably expected to reach acceptable maturity within the project timeframe and resources.
5. Proposed project ICME developments are clearly defined and feasibly achieved within the project timeframe and resources.
6. The project develops methods, models, tools, and standards accessible to the domestic industrial community.
7. The project develops methods, models, tools, and standards that are widely applicable and transportable.
8. The project provides validation and uncertainty metrics for new methods, models, tools, and standards.
9. Project research has a viable approach for overcoming all relevant implementation barriers.
10. The project results in development of a standard practice or procedure that is formally documented by the performing organization.

Such criteria could certainly be used to develop and refine general topic areas as well as specific programs for consideration, in addition to use for evaluation of proposals.

6.4 Proposed Oversight and Coordination Activity:

It is clear that sustained progress and success for ICME will be dependent upon a coordinated, integrated effort amongst the many participants, sponsors, and beneficiaries. Consequently, this is believed to be a critical element of the proposed strategy. Coordination, integration, and oversight can be achieved in many ways. What is proposed here is a simple structure comprised of a steering committee with a sub-committee structure that can be adapted as required.

Guidelines for the recommended integration and oversight activities:

1. Develop a coordinated government – industry steering committee for general oversight, policy definition, and communication. This could be similar to the "HCF Steering Committee" initiated by the USAF during formation and execution of the "HCF Initiative" of the 1990's through early 2000's. The subcommittees recommended below would take guidance from this steering committee.

2. Initiate a subcommittee to determine technical requirements and priorities. This could be similar to the GUIDE Consortium activities for HCF aeroelasticity code development and associated measurement techniques (NSMS), or have a similar structure.
3. Initiate a subcommittee to address standards and integration – focused on software, software modules, compatibility and commercial availability, and standards for data bases and integration of software.
4. Establish a formal policy and procedure for program and task selection and administration. It is possible that this could be done under the direction of AFRL by the MAI association, utilizing the current MAI ESC and TOC structure, or by a similar organization.
5. Establish an additional subcommittee for the academia and small business efforts, with responsibility to define and prioritize SBIR and STTR tasks, coordinate with current agency activities such as AFOSR and ONR, and integrate as appropriate with current university activities in the ICME area.

6.5 Proposed Integration of University and Small Business Activities:

Universities and small businesses have contributed significantly to the current state of ICME and will be critical to future development and long term success. Specific model development activities, and implementation through applicable software will be key areas for their participation. So, it is important to have a sustainable, coordinated plan and activity to engage both universities and small businesses. The proposed strategy is to engage current university sponsors such as AFOSR and ONR, as well as to utilize the SBIR and STTR programs. This requires development of a comprehensive plan for the desired activities and having an "owner" or responsible entity to maintain, market, and oversee the plan. The recommendation is that this be done by the subcommittee defined above.

Guidelines for the coordinated academia and small business activities:

1. Determine requirements and focus areas based on recommendations of the integration and oversight committees previously described.
2. Utilize the SBIR and STTR process and programs where possible – by submitting topics consistent with sponsoring agency requirements that are also aligned with ICME needs and goals.
3. Identify and engage as appropriate the various current agency and university "center of excellence" activities in ICME related activities.
4. Ensure focus on output consistent with commercially available code or code modules which are compatible with currently available and/or broadly used commercial codes.
5. Focus activities on common, broadly used or critical materials.

The descriptions and recommendations presented above were intended to provide sufficient detail to convey the thinking behind the recommended activities, consistent with the strategy that was presented, without overly constraining the specific content of any of the elements. It is expected that considerable discussion and effort may be required to determine the specific projects and actions that would best serve development

and implementation of ICME, and to best match such projects with program and sponsoring agency resources which would benefit.

7. Recommended Next Steps

Previous sections of this white paper have described the current state of ICME and the key challenges and barriers that must be addressed, from the perspective of the authors. A comprehensive general strategy was described, and specific recommendations and guidelines were developed and presented in sufficient detail for initial discussion and program development. The strategy that was presented involved a combination of elements, including several selected industrial projects and focus areas, recommendations for sustained involvement of universities and small businesses, and a recommended approach for oversight and integration of an overall ICME initiative.

Such broad recommendations would, of course, require significant commitment of resources and the involvement of several organizations over a sustained period of years to fully implement. A plan to get such a comprehensive initiative underway in the first place is an important element, and development of a long-term plan is essential.

While development of a long-term plan was beyond the scope of this white paper, a "notional" five-year plan and schedule was developed to facilitate discussion of the activities required to get such an ICME initiative started. This is presented in Figure 4. The figure shows four categories of activities: initial planning and roadmap development, the industrial projects and focus areas, placeholder bars for university and small business activities, and the proposed oversight and integration activities.

The specific next steps that are recommended are summarized below. Initial focus is on development of the strategy and plan under AFRL leadership, followed by securing support from key organizations such as MAI, and then initiating the support structure and consensus-building activities necessary to ensure alignment with and support for the plan. This may include presenting and working the plan with other key organizations in the Navy, DARPA, and NASA as appropriate. These next steps also include two very critical milestones related to both AFRL and MAI – and that is solicitation for two of the identified projects in the key industrial topic areas – specifically ICME for Residual Stress, and ICME for Materials Development. Both are aligned with current and recent MAI and AFRL contractual activities, and both are believed to provide the right opportunity for successful development, application, and validation of ICME methods, where benefits from success will ensure institutionalization.
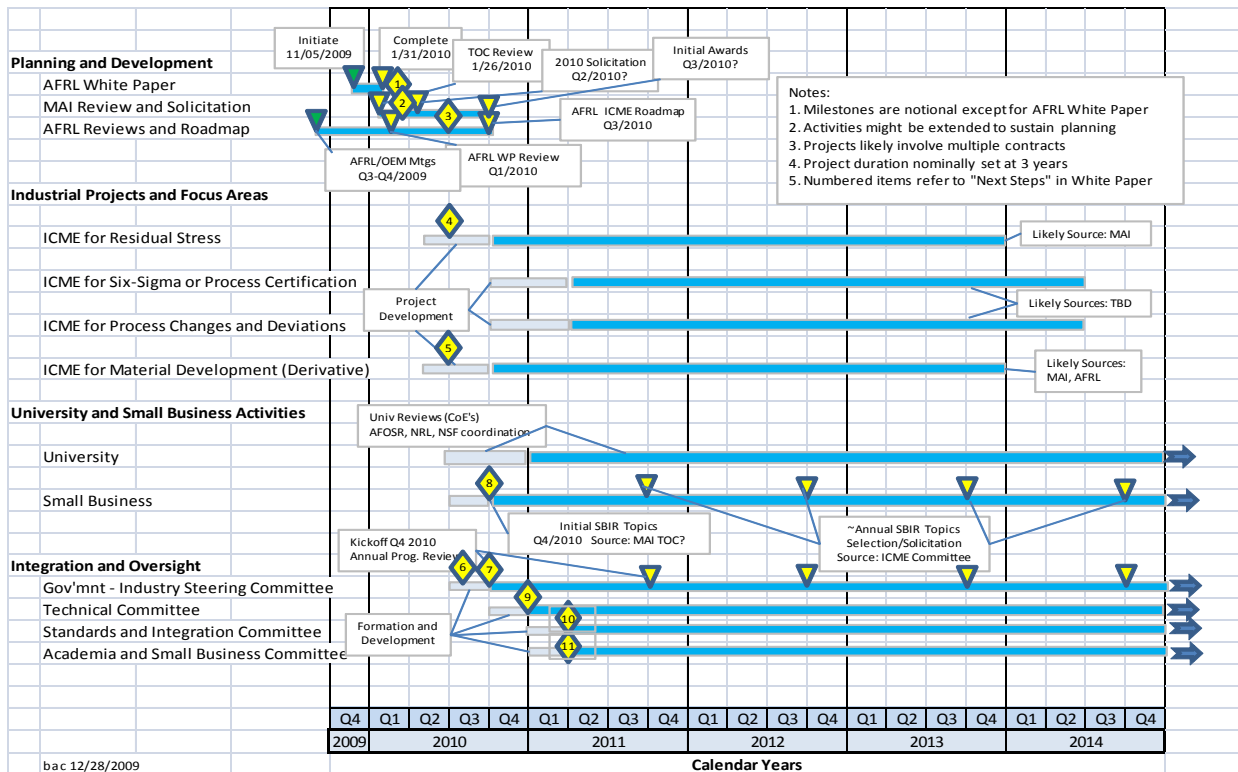
Figure 4: Notional Five-Year Plan and Schedule for Focused ICME Effort

The recommended next steps are listed below:

1. Secure AFRL concurrence and commitment – ie: white paper concept approval/modification
2. Review white paper concepts with MAI and achieve MAI support
3. Develop AFRL Plan and Roadmap
4. MAI/AFRL Commitment for "ICME for Residual Stress" solicitation
5. MAI/AFRL Commitment for "ICME for Material Development (Derivative Material) solicitation - preferably aligned with AFRL/MAI Hybrid Disk programs)
6. Presentation of plan and alignment with other agencies – Navy, DARPA, NASA
7. Initiation of Government-Industry Steering Committee
8. Development of initial SBIR topics and identification of sponsorship agencies
9. Initiate Technical subcommittee
10. Initiate Standards and Integration subcommittee
11. Initiate Academia and Small Business subcommittee

These recommended next steps, along with notional target dates and proposed actionees, are summarized in Table 5, below, and are also indicated by the numbered diamond symbols on the notional five-year plan and schedule presented in Figure 4.

Table 5: Recommended Next Steps, Notional Dates, and Recommended Actionees

"Next Step"	Description	Notional Target Date	Recommended Actionee(s)	Remarks
1	Secure AFRL concurrence and commitment – ie: white paper concept approval/modification	3/15/2010	Consultants and AFRL	
2	Review white paper concepts with MAI and achieve MAI support	2/15/2010	Consultants and AFRL	
3	Develop AFRL Plan and Roadmap	6/1/2010	AFRL	
4	MAI/AFRL Commitment for "ICME for Residual Stress" solicitation	6/15/2010	AFRL and MAI TOC	Projects focused on "bulk" resdidual stresses
5	MAI/AFRL Commitment for "ICME for Material Development (Derivative Material) solicitation	6/15/2010	AFRL and MAI TOC	Projects preferably aligned with AFRL/MAI Hybrid Disk programs
6	Presentation of plan and alignment with other agencies	8/15/2010	AFRL	Navy, DARPA, NASA, possibly FAA
7	Initiation of Government-Industry Steering Committee	10/1/2010	AFRL	Review USAF HCF Steering Committee as possible model
8	Development of initial SBIR topics and identification of sponsorship agencies	9/15/2010	AFRL, MAI and Consultants	
9	Initiate Technical subcommittee	12/31/2010	GI Steering Committee	Review GUIDE consortium as possible model
10	Initiate Standards and Integration subcommittee	3/31/2011	GI Steering Committee	Review FAA - industry RISC and Engine Ti Consortium as possible models
11	Initiate Academia and Small Business subcommittee	3/31/2011	GI Steering Committee	Review current University CoEs, plan SBIR topic approach, contact AFOSR, NRL, etc

8. Summary and Closing Comments

It is believed that substantial cost, schedule, and technical benefits would result from broad development, implementation, and validation of ICME for aerospace applications. It is also believed that such development and implementation is necessary, even essential, to ensure that materials engineering play a significant continuing role in aerospace system design and development. Such capability is especially critical to ensure that the development cycle time for materials and processes be made compatible with the timing and technical requirements for overall system design, optimization, and development. Such ICME capability is also critical for accelerating the schedule and reducing the costs associated with all manner of materials engineering activities: including development of derivative materials and processes, evaluating the effects of intended process changes as well as variations from engineering intent, and the establishment of "Six-sigma" capable and "Certified Processes."

Challenges and barriers are formidable. ICME tools must span and integrate a wide range of physics, materials science, statistics, and even cost models. There are the substantial challenges of model development, generation of requisite supporting data, accuracy, validation, integration, and finally (but by no means least challenging) – acceptance. Yet previous efforts and studies have demonstrated the value and tremendous potential of ICME. Analogous capability is already in routine use by many other aerospace disciplines – where the challenges of model integration, execution, and validation have been successfully addressed. This capability has facilitated the Multi-Discipline Optimization that is critical to future aerospace system development. One can argue that the challenges for materials science and engineering are more wide ranging, less amenable to accurate representation by physics based models, and thus more formidable. But: these challenges should in no way prevent development- and execution - of a long

range plan for ICME. It may require that more empirically-based or phenomenological models be used, that the integration of models with sequential dependencies be carefully assessed or even limited, and that early applications focus on areas where extensive validation may not be necessary. The most immediate requirement for successful initiation of an ICME plan is that we define focus areas with quantifiable benefits – and that we get started.

The focus of this white paper – bearing in mind that it represents one "person-month" of total effort on the part of the authors – was to assess the current state of ICME from a high level perspective, to develop a general strategy, and to define an "actionable" plan for ICME. The intent was not to specify detailed actions or select models for development. Rather, the intent was to provide a basis for detailed discussion amongst the many participants and stakeholders in ICME for development of a long-term roadmap, and hopefully to facilitate commitments from potential sponsors to initiate near-term industrial projects in key focus areas.

If we are successful at launching at least two of the proposed key industrial projects that were defined, we would have the community interest, the credibility, and the momentum to initiate and sustain the proposed planning and oversight activities, as well as to engage the associated and very important support from universities and small businesses.

Demonstration of the value of ICME for sustained investment and development will take time. It will almost certainly occur incrementally – one small step at a time. It is therefore incumbent on the leadership of the materials science and engineering community that the long range view be taken – and that a supporting vision and roadmap be developed. The most immediate requirement for success, we believe, is to define and secure sponsorship for focused projects in critical areas as defined. Development of roadmaps, long range plans, integration and oversight approaches, and supporting efforts can follow closely, once there is evidence of a sustained activity.

The authors hope that this brief study and opinion paper will facilitate the critical next steps.

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